Autoencoders and Restricted Boltzmann Machines

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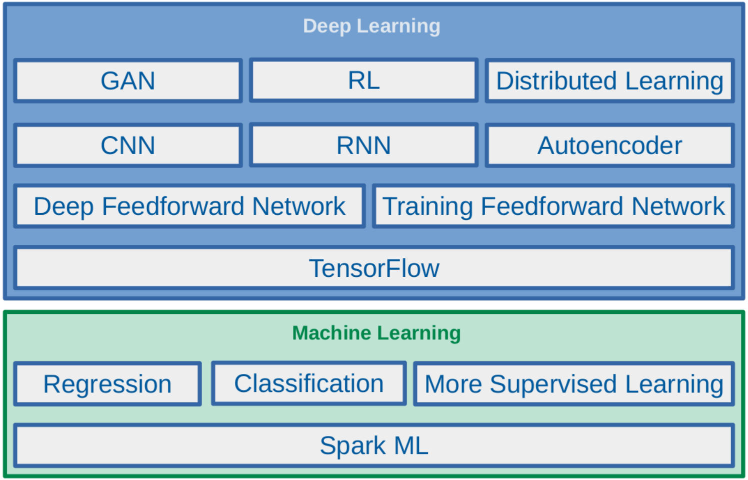
27/11/2019

The Course Web Page

https://id2223kth.github.io

Where Are We?


Deep Learning
GAN
RL
Distributed Learning
CNN
RNN
Autoencoder
Deep Feedforward Network
Training Feedforward Network
TensorFlow
Machine Learning
Regression
Classification
More Supervised Learning
Spark ML

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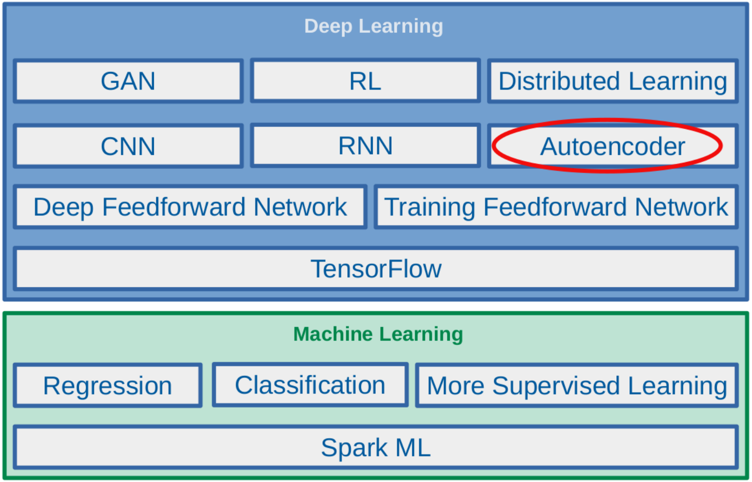

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Let's Start With An Example

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- Seq1 is shorter, so it should be easier.

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- But, Seq2 follows two simple rules:

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  - Even numbers are followed by their half.
  - Odd numbers are followed by their triple plus one.

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- You don't need pattern if you could quickly and easily memorize very long sequences
- But, it is hard to memorize long sequences that makes it useful to recognize patterns.

- 1970, W. Chase and H. Simon
- They observed that expert chess players were able to memorize the positions of all the pieces in a game by looking at the board for just 5 seconds.

- This was only the case when the pieces were placed in realistic positions, not when the pieces were placed randomly.

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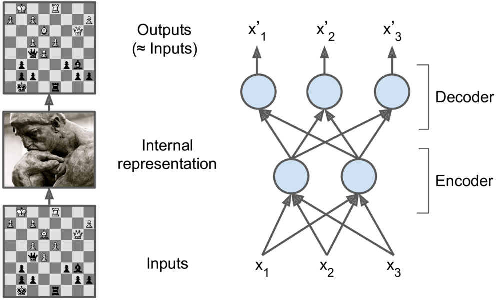
- They just see chess patterns more easily due to their experience with the game.
- Patterns helps them store information efficiently.

Autoencoders

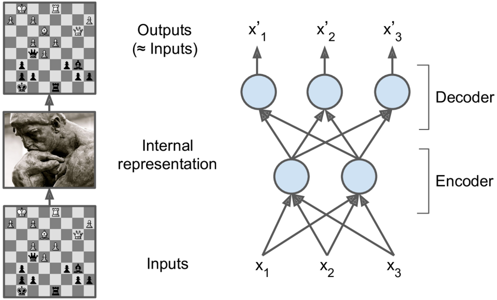
Autoencoders (1/5)

- Just like the chess players in this memory experiment.



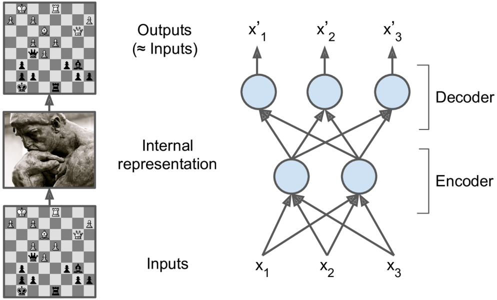
Autoencoders (1/5)

- Just like the chess players in this memory experiment.
- An autoencoder looks at the inputs, converts them to an efficient internal representation, and then spits out something that looks very close to the inputs.



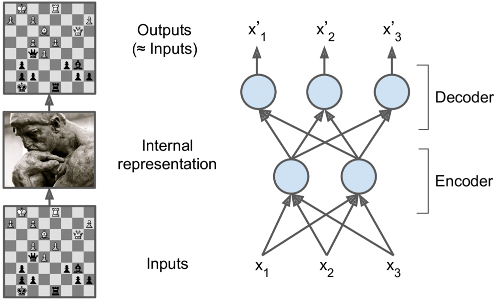
Autoencoders (2/5)

- The same architecture as a Multi-Layer Perceptron (MLP).



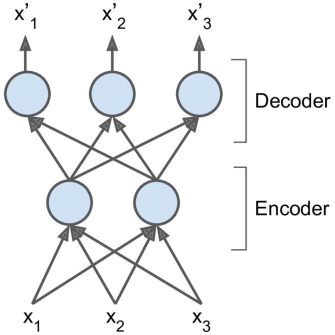
Autoencoders (2/5)

- The same architecture as a Multi-Layer Perceptron (MLP).
- Except that the number of neurons in the output layer must be equal to the number of inputs.



Autoencoders (3/5)

- An autoencoder is always composed of two parts.



Autoencoders (3/5)

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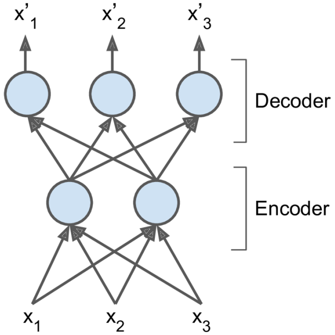
- An encoder (recognition network), $\mathbf{h} = \mathtt{f}(\mathbf{x})$
  Converts the inputs to an internal representation.



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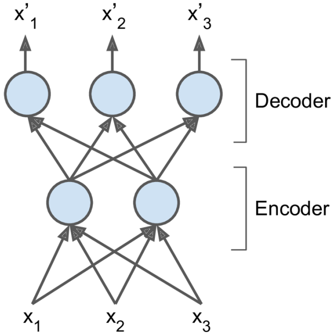

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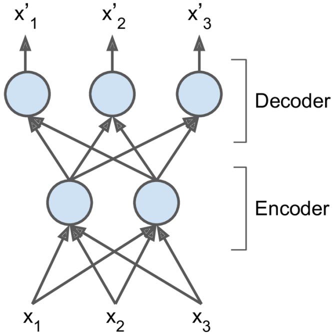
  Converts the inputs to an internal representation.
- A decoder (generative network), $\mathbf{r} = \mathrm{g}(\mathbf{h})$
  Converts the internal representation to the outputs.
- If an autoencoder learns to set $\mathrm{g}(\mathtt{f}(\mathbf{x})) = \mathbf{x}$ everywhere, it is not especially useful, why?



Autoencoders (4/5)

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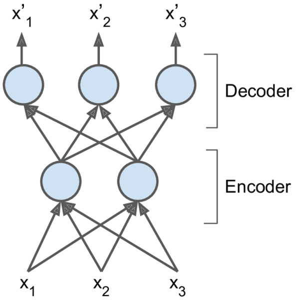
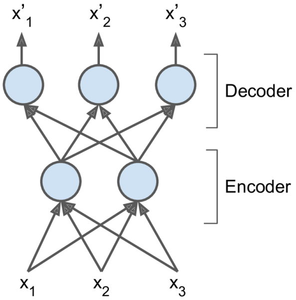


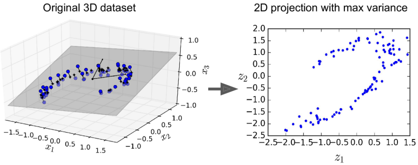
Autoencoders (4/5)

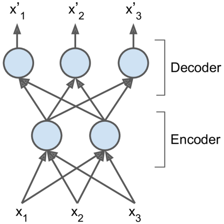
- Autoencoders are designed to be unable to learn to copy perfectly.
- The models are forced to prioritize which aspects of the input should be copied, they often learn useful properties of the data.



Autoencoders (5/5)

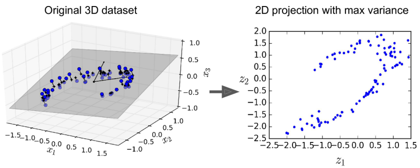
- Autoencoders are neural networks capable of learning efficient representations of the input data (called codings) without any supervision.

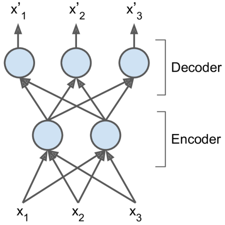




Autoencoders (5/5)

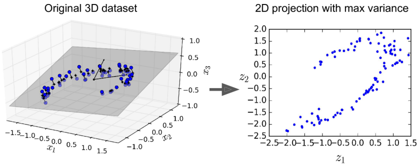
- Autoencoders are neural networks capable of learning efficient representations of the input data (called codings) without any supervision.
- Dimension reduction: these codings typically have a much lower dimensionality than the input data.

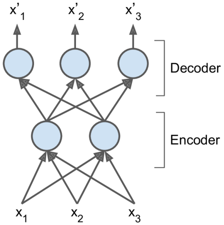




Dimension Reduction and PCA

- Principal Component Analysis (PCA) is the most popular dimensionality reduction algorithm.





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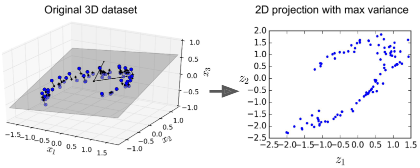

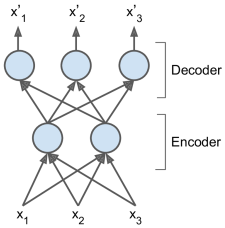

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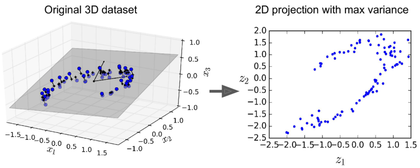
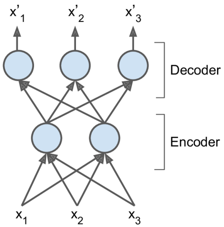
- Autoencoders with nonlinear encoder and decoder functions can thus learn a more powerful nonlinear generalization of PCA.





PCA with an Undercomplete Linear Autoencoder

- A linear autoencoder to perform PCA on a 3D dataset, projecting it to 2D.

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n_inputs = 3  # 3D inputs
n_hidden = 2  # 2D codings
n_outputs = n_inputs
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```
encoder = keras.models.Sequential([keras.layers.Dense(n_hidden, input_shape=[n_inputs])])
decoder = keras.models.Sequential([keras.layers.Dense(n_outputs, input_shape=[n_hidden])])
autoencoder = keras.models.Sequential([encoder, decoder])

autoencoder.compile(loss="mse", optimizer=keras.optimizers.SGD(lr=1.5))
```

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Stacked Autoencoders (1/3)

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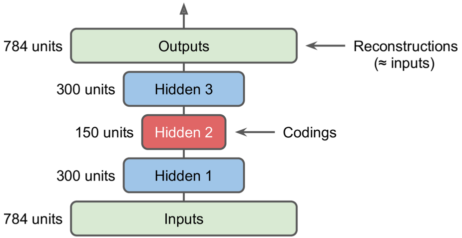

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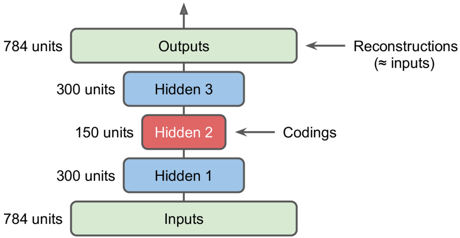
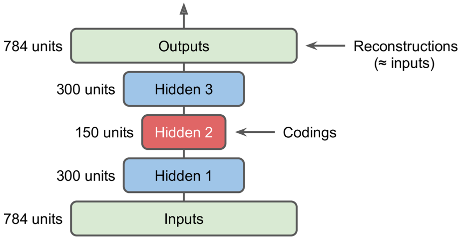


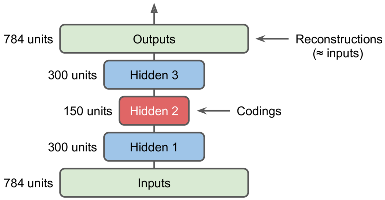
Stacked Autoencoders (1/3)

- Stacked autoencoder: autoencoders with multiple hidden layers.
- Adding more layers helps the autoencoder learn more complex codings.
- The architecture is typically symmetrical with regards to the central hidden layer.



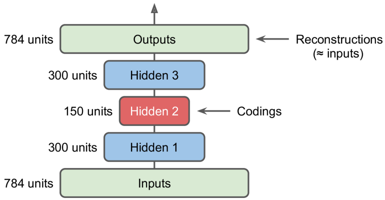
Stacked Autoencoders (2/3)

- In a symmetric architecture, we can tie the weights of the decoder layers to the weights of the encoder layers.



Stacked Autoencoders (2/3)

- In a symmetric architecture, we can tie the weights of the decoder layers to the weights of the encoder layers.
- In a network with $\mathtt{N}$ layers, the decoder layer weights can be defined as $\mathtt{w}_{\mathtt{N}-\mathtt{l}+1} = \mathtt{w}_{\mathtt{l}}^{\mathtt{T}}$, with $\mathtt{l} = 1, 2, \cdots, \frac{\mathtt{N}}{2}$.



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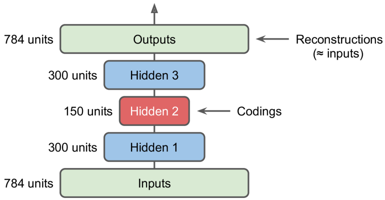
- This halves the number of weights in the model, speeding up training and limiting the risk of overfitting.



Stacked Autoencoders (3/3)

```
stacked_encoder = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[28, 28]),
    keras.layers.Dense(100, activation="relu"),
    keras.layers.Dense(30, activation="relu"),
])
stacked_decoder = keras.models.Sequential([
    keras.layers.Dense(100, activation="relu", input_shape=[30]),
    keras.layers.Dense(28 * 28, activation="sigmoid"),
    keras.layers.Reshape([28, 28])
])
stacked_ae = keras.models.Sequential([stacked_encoder, stacked_decoder])
```

Different Types of Autoencoders

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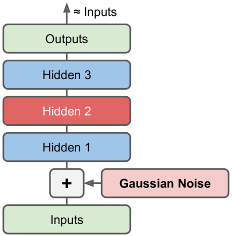
Denoising Autoencoders (1/3)

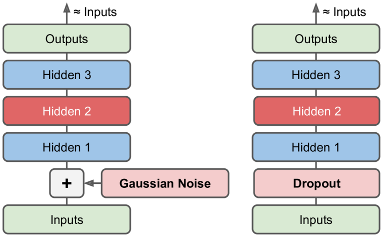
- One way to force the autoencoder to learn useful features is to add noise to its inputs, training it to recover the original noise-free inputs.



Denoising Autoencoders (1/3)

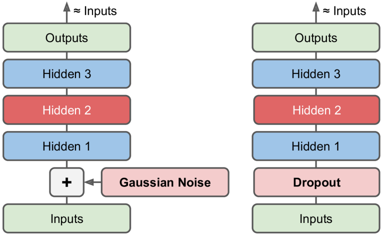
- One way to force the autoencoder to learn useful features is to add noise to its inputs, training it to recover the original noise-free inputs.

- This prevents the autoencoder from trivially copying its inputs to its outputs, so it ends up having to find patterns in the data.



Denoising Autoencoders (2/3)

- The noise can be pure Gaussian noise added to the inputs, or it can be randomly switched off inputs, just like in dropout.



Denoising Autoencoders (3/3)

```
denoising_encoder = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[28, 28]),
    keras.layers.GaussianNoise(0.2),
    keras.layers.Dense(100, activation="relu"),
    keras.layers.Dense(30, activation="relu")
])
denoising_decoder = keras.models.Sequential([
    keras.layers.Dense(100, activation="relu", input_shape=[30]),
    keras.layers.Dense(28 * 28, activation="sigmoid"),
    keras.layers.Reshape([28, 28])
])
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  - As opposed to denoising autoencoders, which use randomness only during training.

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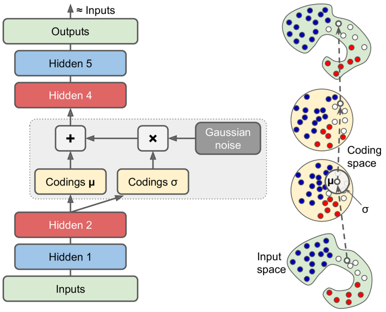
- Their outputs are partly determined by chance, even after training.
  - As opposed to denoising autoencoders, which use randomness only during training.
- They are generative autoencoders, meaning that they can generate new instances that look like they were sampled from the training set.

Variational Autoencoders (2/3)

- Instead of directly producing a coding for a given input, the encoder produces a mean coding μ and a standard deviation σ.



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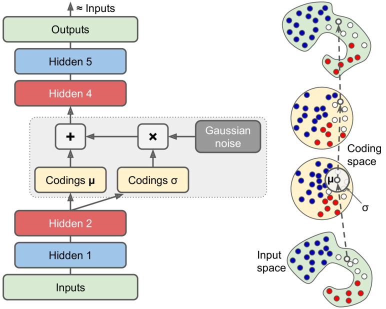
- The actual coding is then sampled randomly from a Gaussian distribution with mean μ and standard deviation σ.



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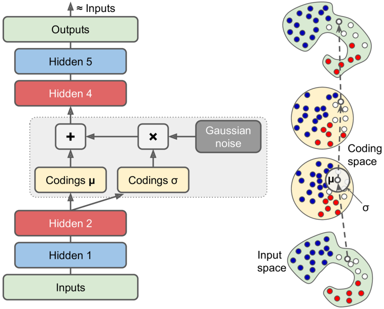
- The actual coding is then sampled randomly from a Gaussian distribution with mean μ and standard deviation σ.
- After that the decoder just decodes the sampled coding normally.



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  - Pushes the autoencoder to have codings that look as though they were sampled from a simple Gaussian distribution.
  - Using the KL divergence between the target distribution (the Gaussian distribution) and the actual distribution of the codings.
  - KL divergence measures the divergence between the two probabilities.


$S = k \log W$
Original illustration: Sonia Jerrems

Restricted Boltzmann Machines

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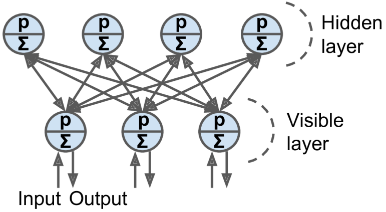
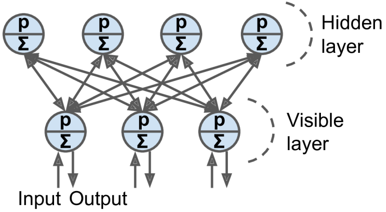
- A Restricted Boltzmann Machine (RBM) is a stochastic neural network.



Restricted Boltzmann Machines

- A Restricted Boltzmann Machine (RBM) is a stochastic neural network.
- Stochastic meaning these activations have a probabilistic element, instead of deterministic functions, e.g., logistic or ReLU.



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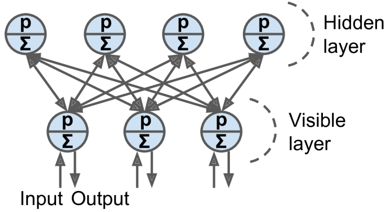
- Stochastic meaning these activations have a probabilistic element, instead of deterministic functions, e.g., logistic or ReLU.
- The neurons form a bipartite graph:
  - One visible layer and one hidden layer.
  - A symmetric connection between the two layers.
  - There are no connections between neurons within a layer.



Let's Start With An Example

RBM Example (1/10)

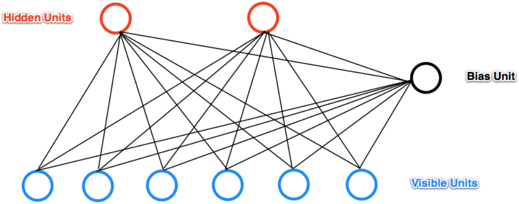
- We have a set of six movies, and we ask users to tell us which ones they want to watch.

RBM Example (1/10)

- We have a set of six movies, and we ask users to tell us which ones they want to watch.
- We want to learn two latent neurons (hidden neurons) underlying movie preferences, e.g., SF/fantasy and Oscar winners

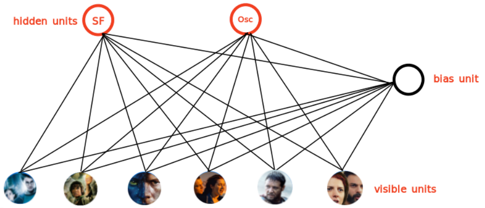
RBM Example (2/10)

- Our RBM would look like the following.



RBM Example (3/10)

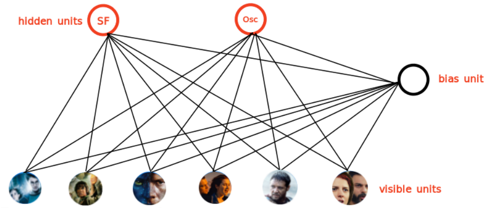
- Assume the given input x_i is the 0 or 1 for each visible neuron v_i.
  - 1: like a movie, and 0: dislike a movie



RBM Example (3/10)

- Assume the given input x_i is the 0 or 1 for each visible neuron v_i.
  - 1: like a movie, and 0: dislike a movie
- Compute the activation energy at hidden neuron h_j:

$$a(h_j) = \sum_i w_{ij} v_i$$

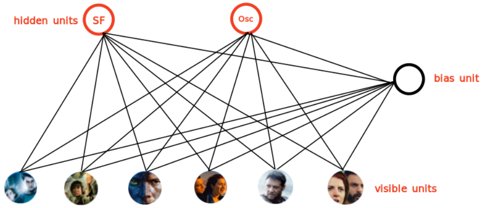


RBM Example (4/10)

- For each hidden neuron $\mathtt{h_j}$, we compute the probability $\mathtt{p(h_j)}$.

$$a(h_j) = \sum_i w_{ij} v_i$$

$$p(h_j) = \text{sigmoid}(a(h_j)) = \frac{1}{1 + e^{-a(h_j)}}$$



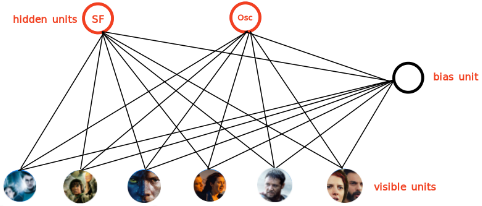
RBM Example (4/10)

- For each hidden neuron $\mathtt{h_j}$, we compute the probability $\mathtt{p(h_j)}$.

$$\mathtt{a(h_j)} = \sum_{\mathtt{i}} \mathtt{w_{ij} v_i}$$

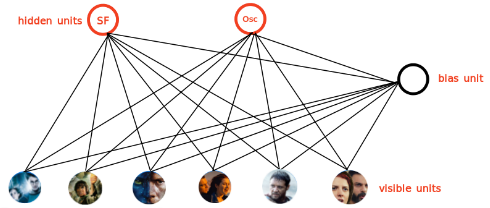
$$\mathtt{p(h_j)} = \mathtt{sigmoid(a(h_j))} = \frac{1}{1 + \mathtt{e}^{-\mathtt{a(h_j)}}}$$

- We turn on the hidden neuron $\mathtt{h_j}$ with the probability $\mathtt{p(h_j)}$, and turn it off with probability $1 - \mathtt{p(h_j)}$.



RBM Example (5/10)

- Declaring that you like Harry Potter, Avatar, and LOTR, doesn't guarantee that the SF/fantasy hidden neuron will turn on.



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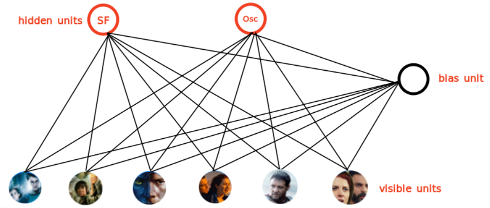
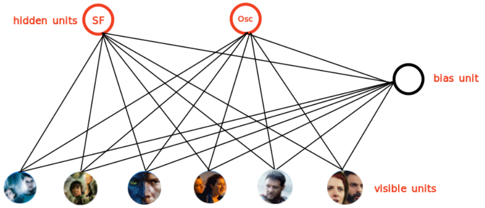


RBM Example (5/10)

- Declaring that you like Harry Potter, Avatar, and LOTR, doesn't guarantee that the SF/fantasy hidden neuron will turn on.
- But it will turn on with a high probability.
  - In reality, if you want to watch all three of those movies makes us highly suspect you like SF/fantasy in general.
  - But there's a small chance you like them for other reasons.



RBM Example (6/10)

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- The hidden neurons send messages to the visible (movie) neurons, telling them to update their states.

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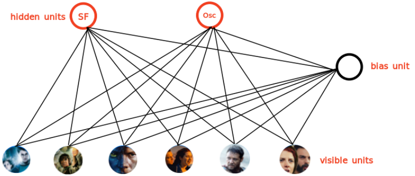
- Being on the SF/fantasy neuron doesn't guarantee that we'll always recommend all three of Harry Potter, Avatar, and LOTR.
  - For example not everyone who likes science fiction liked Avatar.

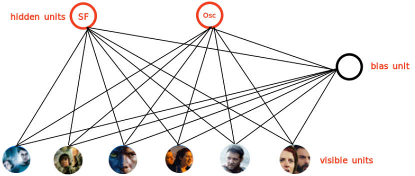
RBM Example (7/10)

- How do we learn the connection weights w_{ij} in our network?



RBM Example (7/10)

- How do we learn the connection weights $\mathtt{w_{ij}}$ in our network?
- Assume, as an input we have a bunch of binary vectors $\mathbf{x}$ with six elements corresponding to a user's movie preferences.



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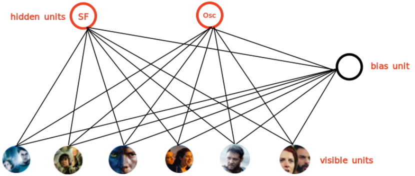

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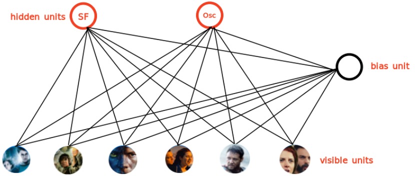
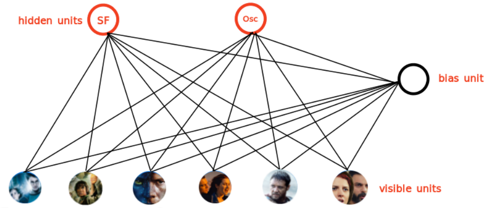
- How do we learn the connection weights w_{ij} in our network?
- Assume, as an input we have a bunch of binary vectors $\mathbf{x}$ with six elements corresponding to a user's movie preferences.
- We do the following steps in each epoch:
- 1. Take a training instance $\mathbf{x}$ and set the states of the visible neurons to these preferences.



RBM Example (8/10)

- 2. Update the states of the hidden neurons.



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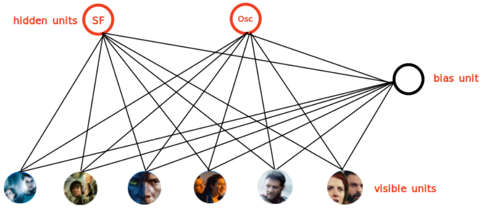

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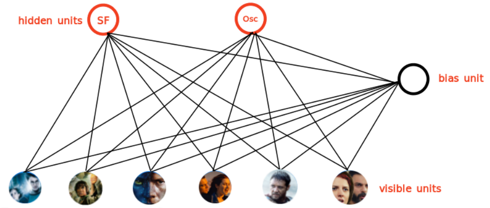

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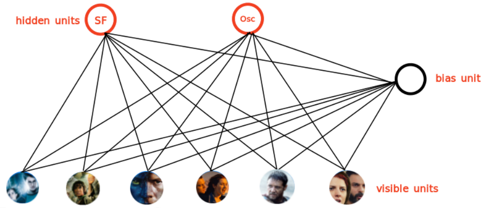
- 3. For each edge $\mathtt{e}_{\mathtt{ij}}$, compute $\mathtt{positive}(\mathtt{e}_{\mathtt{ij}}) = \mathtt{v}_\mathtt{i} \times \mathtt{h}_\mathtt{j}$
  - I.e., for each pair of neurons, measure whether they are both on.



RBM Example (9/10)

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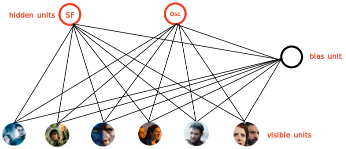

RBM Example (9/10)

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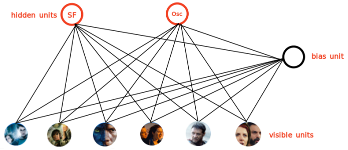

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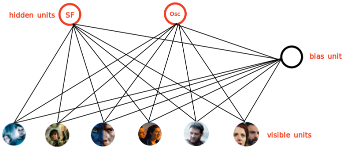

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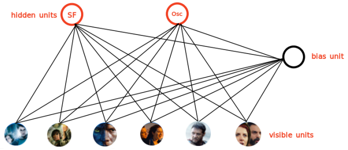
- 5. Update the hidden neurons again similar to step 2. We denote the updated hidden neurons with $\mathtt{h}'_\mathtt{j}$.



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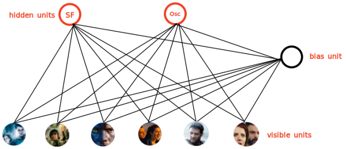
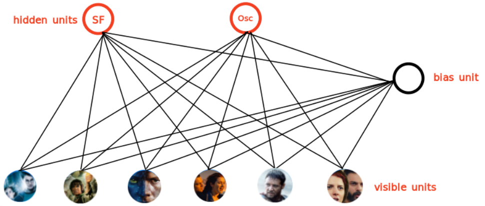
- 5. Update the hidden neurons again similar to step 2. We denote the updated hidden neurons with $\mathtt{h}'_\mathtt{j}$.
- 6. For each edge $\mathtt{e}_{\mathtt{ij}}$, compute $\mathtt{negative}(\mathtt{e}_{\mathtt{ij}}) = \mathtt{v}'_\mathtt{i} \times \mathtt{h}'_\mathtt{j}$



RBM Example (10/10)

- 7. Update the weight of each edge $\mathtt{e_{ij}}$.

$$\mathtt{w_{ij}} = \mathtt{w_{ij}} + \eta(\mathtt{positive}(\mathtt{e_{ij}}) - \mathtt{negative}(\mathtt{e_{ij}}))$$



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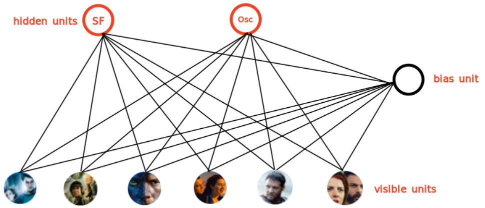
- 8. Repeat over all training examples.



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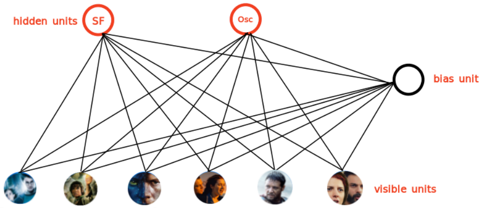
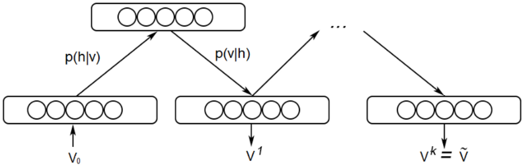
- 9. Continue until the error between the training examples and their reconstructions falls below some threshold or we reach some maximum number of epochs.



RBM Training (1/2)

- Step 1, Gibbs sampling: what we have done in steps 1-6.



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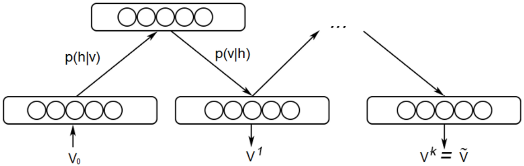
- Given an input vector $\mathbf{v}$, compute $p(\mathbf{h}|\mathbf{v})$.



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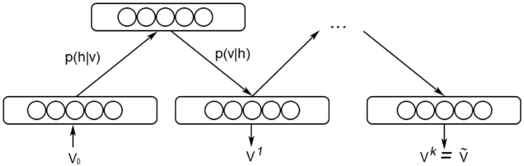
- Knowing the hidden values $\mathbf{h}$, we use $p(\mathbf{v}|\mathbf{h})$ for prediction of new input values $\mathbf{v}$.



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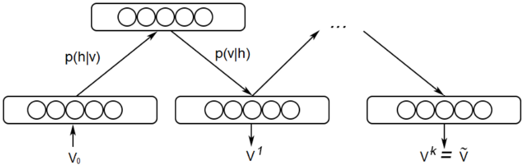
- This process is repeated $\mathtt{k}$ times.



RBM Training (2/2)

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$$
\begin{aligned}
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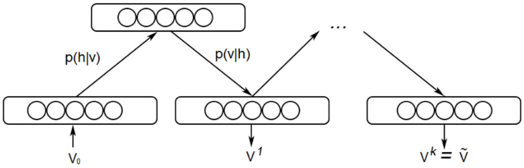

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$$\texttt{positive}(\mathbf{e}) = \mathbf{v}_0 \times p(\mathbf{h}_0|\mathbf{v}_0)$$
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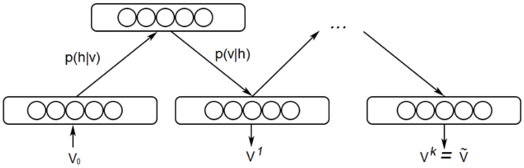
$$\mathbf{w} = \mathbf{w} + \eta(\texttt{positive}(\mathbf{e}) - \texttt{negative}(\mathbf{e}))$$

- $\mathbf{v}_0$ is the original input, and $\mathbf{v}_\mathtt{k}$ is the input after $\mathtt{k}$ iterations.



More Details about RBM

Energy-based Model (1/3)

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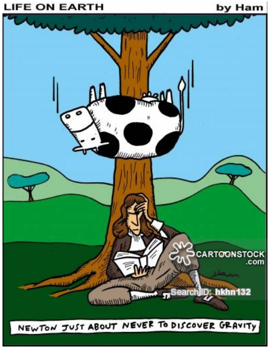
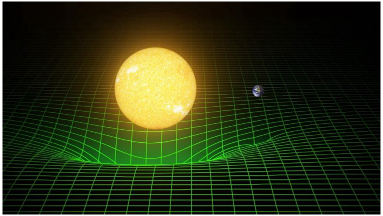
  - E.g., gravitational energy describes the potential energy a body with mass has in relation to another massive object due to gravity.



Energy-based Model (2/3)

- One purpose of deep learning models is to encode dependencies between variables.



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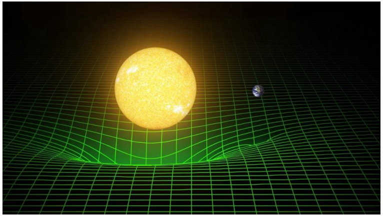

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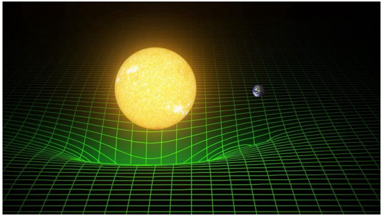
- A high energy means a bad compatibility.



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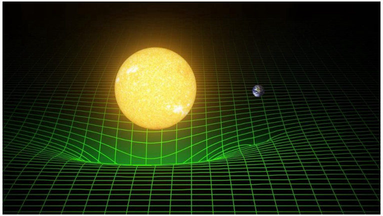
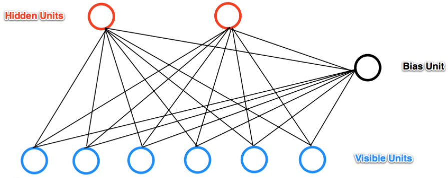
- One purpose of deep learning models is to encode dependencies between variables.
- The capturing of dependencies happen through associating of a scalar energy to each state of the variables.
  - Serves as a measure of compatibility.
- A high energy means a bad compatibility.
- An energy based model tries always to minimize a predefined energy function.



Energy-based Model (3/3)

- The energy function for the RBMs is defined as:

$$E(\mathbf{v}, \mathbf{h}) = -(\sum_{ij} w_{ij} v_i h_j + \sum_{i} b_i v_i + \sum_{j} c_j h_j)$$



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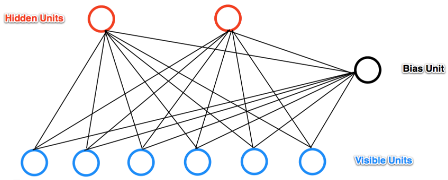
- $\mathbf{v}$ and $\mathbf{h}$ represent the visible and hidden units, respectively.



Energy-based Model (3/3)

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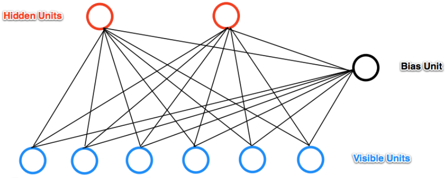

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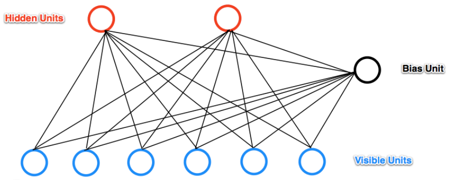
- $\mathbf{b}$ and $\mathbf{c}$ are the biases of the visible and hidden layers, respectively.



RBM Is A Probabilistic Model (1/2)

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- As in Physics we assign a probability to observe a state of $\mathbf{v}$ and $\mathbf{h}$, that depends on the overall energy of the model E.
- At each point in time the RBM is in a certain state.
  - The state refers to the values of neurons in the visible and hidden layers $\mathbf{v}$ and $\mathbf{h}$.

RBM is a Probabilistic Model (2/2)

- The probability of a certain state of $\mathbf{v}$ and $\mathbf{h}$:

$$p(\mathbf{v}, \mathbf{h} | \mathbf{w}) = \frac{e^{-E(\mathbf{v}, \mathbf{h})}}{\sum_{\mathbf{v}, \mathbf{h}} e^{-E(\mathbf{v}, \mathbf{h})}}$$

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- The probability that the network assigns to a visible vector $\mathbf{v}$, is given by summing over all possible hidden vectors $\mathbf{h}$.

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- Use the maximum-likelihood estimation.
- For a model of the form $p(\mathbf{v})$ with parameters $\mathbf{w}$, the log-likelihood given a single training example $\mathbf{v}$ is:

$$\log p(\mathbf{v}|\mathbf{w}) = \log \frac{\sum_{\mathbf{h}} e^{-E(\mathbf{v},\mathbf{h})}}{\sum_{\mathbf{v},\mathbf{h}} e^{-E(\mathbf{v},\mathbf{h})}} = \log \sum_{\mathbf{h}} e^{-E(\mathbf{v},\mathbf{h})} - \log \sum_{\mathbf{v},\mathbf{h}} e^{-E(\mathbf{v},\mathbf{h})}$$

Learning in Boltzmann Machines (2/2)

- The log-likelihood gradients for an RBM with binary units:

$$\frac{\partial \log p(\mathbf{v}|\mathtt{w_{ij}})}{\partial \mathtt{w_{ij}}} = \mathtt{positive}(\mathtt{e_{ij}}) - \mathtt{negative}(\mathtt{e_{ij}})$$

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- Then, we can update the weight **w** as follows:

$$\mathtt{w}_{\mathtt{ij}}^{(\mathtt{next})} = \mathtt{w_{ij}} + \eta(\mathtt{positive}(\mathtt{e_{ij}}) - \mathtt{negative}(\mathtt{e_{ij}}))$$


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IT'S FINALLY OVER
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Summary

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- Autoencoders
  - Stacked autoencoders
  - Denoising autoencoders
  - Variational autoencoders
- Restricted Boltzmann Machine
  - Gibbs sampling
  - Contrastive divergence

Reference

- Ian Goodfellow et al., Deep Learning (Ch. 14, 20)
- Aurélien Géron, Hands-On Machine Learning (Ch. 15)

Questions?